Abstract Submitted
for the MAR12 Meeting of
The American Physical Society

Theoretical modelling of exchange interactions in metal-phthalocyanines WEI WU, Department of Materials, Imperial College London, ANDREW FISHER, Department of physics and astronomy, University College London, NIC HARRISON, Department of Chemistry, Imperial College London, MICHELE SERRI, ZHENLIN WU, SANDRINE HEUTZ, Department of Materials, Imperial College London, TIM JONES, Department of Chemistry, Warwick University,UK, GABRIEL AEPPLI, Department of physics and astronomy, University College London, ORGANIC SPINTRONICS TEAM — The theoretical understanding of exchange interactions in organics provides a key foundation for quantum molecular magnetism. Recent SQUID magnetometry of a well know organic semiconductor, copper-phthalocyanine [1,2] (CuPc) shows that it forms quasi-one-dimensional spin chains. Green's function perturbation theory calculation [3] is used to find the dominant exchange mechanism. Hybrid density functional theory simulations [4] give a quantitative insight to exchange interactions and electronic structures. Both calculations are performed for different stacking and sliding angles for lithium-Pc, cobalt-Pc, chromium-Pc, and copper-Pc. The exchange interactions depend strongly on stacking angles, but weakly on sliding angles. Our results qualitatively agree with the experiments, and remarkably α-cobalt-Pc has a very large exchange above liquid-Nitrogen temperature. Our theoretical predictions on the exchange interactions can guide experimentalists to design novel organic semiconductors.
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Wei Wu
Department of Materials, Imperial College London

Date submitted: 01 Nov 2011 Electronic form version 1.4